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Evaluating O3 Predictions from a Test Application of the EPA Regional Oxidant Model

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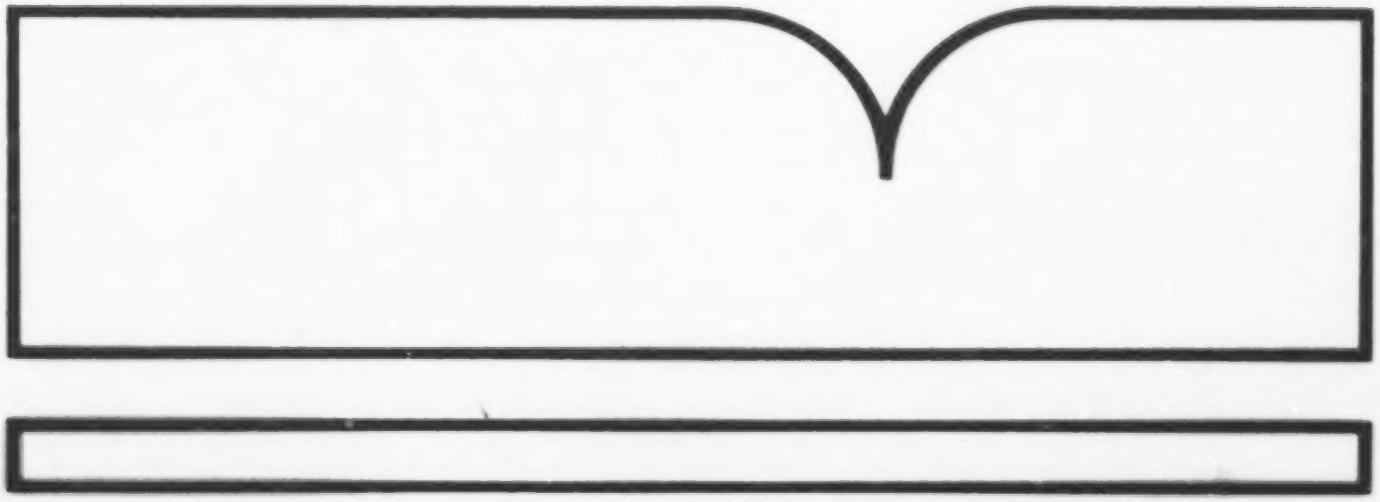

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EVALUATING O_3 PREDICTIONS FROM A TEST APPLICATION OF THE EPA REGIONAL OXIDANT MODEL

by

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16. ABSTRACT

The first generation U.S. EPA Regional Oxidant Model (ROM1) has been tested and evaluated for O_3 predictions on a two-day test case episode (3-4 August 1979) in the Northeast Regional Oxidant Study (NEROS) area. The two-day episode was characterized by relatively high O_3 concentrations in the southern Great Lakes area where clear skies persisted. Intermittent periods of relatively high O_3 levels existed near some of the eastern seaboard cities where partly cloudy skies alternated with clouds and showers in the vicinity of a stationary frontal zone. Model evaluation results for O_3 are presented in two stages. First an analysis of model predictions at all hours of the simulation for all surface monitoring site locations is performed. Results show an average underprediction of only a few percent. In the second stage, an analysis of the ability of the ROM1 to predict daily maximum concentrations, two aspects are considered in the evaluation analysis. First, the maximum O_3 concentrations at monitoring station locations are paired with the corresponding model predictions. Second, the model predictions are analyzed for individual urban emissions source-area plumes.

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1. INTRODUCTION

The U.S. EPA's Regional Oxidant Model (ROM) has been under development and testing for a number of years (Lamb, 1983, 1984; Lamb and Laniak, 1985). The ROM attempts to simulate all of the important physical and chemical processes that affect the generation and dispersion of photochemical smog on regional scales (up to 1000 km). In the present configuration of the ROM domain, the model's horizontal resolution is approximately 18.5 km. In the vertical there are 3 1/2 layers. The first and second layers encompass most of the planetary boundary layer above the surface of the earth and the third layer is the cloud layer extending from cloud base to near the tops of any cumulus-type clouds. Layer 0 is a shallow layer adjacent to the surface designed to treat sub-grid scale effects in the ROM. It is handled in a diagnostic manner within the model.

The model domain used in the first ROM application in the Northeast U.S. included areas covered by special field monitoring projects during the summers of 1979 and 1980. During these projects, highly resolved air quality, meteorological, and source emissions data bases were developed for the study area, hereafter referred to as the NEROS region (Northeast Regional Oxidant Study). The extent of the ROM domain in the NEROS application was 60 cells in the E-W direction and 42 cells in the N-S direction. The dimensions of each individual grid cell were 15 minutes longitude (E-W) and 10 minutes latitude (N-S), or about 18.5 km square cells. The specific episode studied here occurred during 3-4 August 1979, during the first NEROS field project.

The first generation model (ROM1) was the version used in this modeling study. It is a preliminary version with simplified chemistry and a grid cell structure that does not allow for individual cell volumes to change in time. The relevant vertical dimensions are 40 m for layer 0, 400 m for layer 1, 800 m for layer 2, and 800 m for layer 3. This paper discusses the evaluation of ROM1 results for O_3 predictions on the 3-4 August 1979 episode in the NEROS region. The evaluation has been structured in a manner designed to elicit the ROM1's performance for prediction of hourly and maximum O_3 concentrations. The evaluation procedure includes several levels of analysis.

The analysis explores the comparison between ambient O_3 observations and the model-predicted concentrations. First, paired comparisons are made for all hourly observations at all monitoring sites. This analysis brings out gross features of model performance including any systematic features of model bias. Subsets of the full data set are used to explore particular aspects of the comparisons. Next, comparisons are made between maximum daily O_3 concentrations at surface monitoring sites and model predictions of O_3 maxima. These comparisons are performed in a number of ways. (1) Daily maxima at all surface monitoring sites are matched with model predictions at those locations. (2) To isolate the model performance for a given source area, O_3 plumes are individually identified, and the model's ability to predict maximum O_3 concentrations within the plume is evaluated. The two types of maximum value analyses are necessary for assessing the ROM1 as a tool for emission control strategy assessment. Examining all daily O_3 maximum values together illustrates the potential effects a control strategy may have on the entire region. On the other hand, examination of individual plumes will highlight effects of a control strategy on O_3 reductions in a particular urban source area.

2. DATA BASE

Approximately 200 SAROAD air monitoring sites measure hourly ambient O_3 within the NEROS region, although at any given day and hour only a subset of these sites is actively measuring O_3 levels. The surface stations, shown in Fig. 1, are not distributed evenly across the region. They tend to be clustered in the vicinity of urban areas, leaving large portions of the model domain with little or no surface monitored O_3 data. Scarcity of data is especially a problem in the region stretching from the Ohio Valley northeast through central and northern New York state, except for the Pittsburgh area. Model performance in the central section of the grid will therefore be difficult to judge, except in a gross sense. The Northeast corridor of cities is well represented, as is, to a lesser degree, the industrialized areas near the Great Lakes.

The 3-4 August 1979 period was not a major episode for 03, although values exceeded 100 ppb

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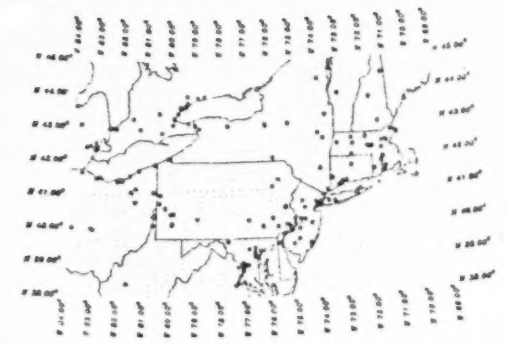

Figure 1. ROM grid resolution in the NEROS study region. O_3 monitoring stations operating during the 3-4 August 1979 period are indicated by dots.

in selected areas. On 3 August, despite the cloud cover and intermittent rain showers over parts of the mid-Atlantic seaboard some O_3 values reached between 100 and 115 ppb in the Washington and Philadelphia areas and between 120 and 130 ppb in the New Jersey, New York and Connecticut area, where there was less cloud cover on that day. The highest O_3 values occurred near the southeast shore of Lake Erie, where Conneaut, Ohio recorded 159 ppb as the daily maximum. On 4 August, the overcast and rainy conditions along the Atlantic coast from New York northward did, in fact, seem to suppress O_3 generation. South of New York, however, relatively high levels were measured near the Philadelphia area (143 ppb) and Washington, D.C. (139 ppb), where skies had cleared. Several observation stations along the south shore of Lake Erie reported maximum O_3 levels from 120 to 135 ppb. Most other areas of the NEROS region reported low values, except for a few observations near 100 ppb downwind of Detroit and Toronto. Aircraft sampling during this 2-day episode over the NEROS region indicated widespread boundary layer O_3 levels of 70 to 80 ppb with some areas slightly higher or lower than this range at times (Clarke and Ching, 1983).

3. RESULTS

The ROM1 was run for the 48-h period of 3-4 August 1979 using data from the NEROS and SAROAD data bases. The model was initialized throughout its entire domain with a set of "clean" tropospheric background species concentrations that were computationally adjusted for chemical equilibrium. The same set of concentrations was used for both lateral inflow and top boundary concentrations throughout the model simulation period. We ignore the first 6 hours of predictions from the model because of the strong influence of initial conditions in this period.

The hourly comparisons of surface O_3 observations and model predictions over all receptor sites and all hours showed that the diurnal range in O_3 concentrations was considerably greater for the actual observations than for the model predictions, where an average variation of only 10 to 15 ppb was shown. Bias values, or observed minus predicted concentration values, were generally negative at night and positive during the day. The average episodic value of observed O_3 for all hours at the surface monitoring sites was 38.9 ppb, and the corresponding model predictions for ROM1 layers 0 and 1 were 36.6 and 38.1 ppb, respectively. These values represent a 5.9% underprediction for layer 0 and a 2.1% underprediction for layer 1. Since these average O_3 levels are near tropospheric background values, there is not a high degree of significance in this analysis over all hourly values.

The next step in the evaluation was to perform an hourly analysis with a subset of the data values already used. The criterion for choosing the subset was based, in part, on the tropospheric background value of approximately 40 ppb O_3 used in the ROM1's initial and boundary conditions and the fact that many of the surface monitoring site locations showed O_3 predictions near this value. Therefore, the data subset was based on only those receptor points for which the observed value and the level 0 and 1 predicted values of O_3 were greater than 50 ppb. This should limit the data to those sites most affected by source emissions within the NEROS region. In fact, after this criterion was applied the number of sites used in the analysis dropped from near 150 during the midday hours to approximately 30, and from around 120 during the nighttime hours to 0.

The analysis of the data subset showed that the average observed concentration at the receptor locations varied from 51.0 ppb at 2000 h to 78.0 ppb at 1300 h on 3 August, and from 50.0 ppb at 0400 h to 80.7 ppb at 1600 h on 4 August. The corresponding predictions for layer 0 ranged from 56.0 ppb at 1900 h to 70.4 ppb at 1600 h on 3 August, and from 54.4 ppb at 0400 h to 76.2 ppb at 2000 h on 4 August. The average episodic value of observed O_3 in the data subset for all hours was 72.2 ppb, and the corresponding ROM1 predictions for layers 0 and 1 were 68.9 and 71.2 ppb, respectively. This represents an average O_3 underprediction of 4.6% for ROM1 layer 0 and 1.4% for layer 1, a slightly smaller degree of underprediction than the values computed for the full data set. The average values in the data subset were however, significantly greater than the tropospheric background O_3 value.

The most significant parameter of interest for the air quality policymaker concerning ambient O_3 is the daily maximum hourly value observed at a monitoring station. The model evaluation for maximum O_3 concentration took place in two steps. First, in the daily maxima analysis by site, model predictions of maximum hourly O_3 levels at surface monitoring site locations were compared with measured values at the sites. Second, in the plume maxima analysis, the concentration magnitudes and position of plumes of O_3 within the NEROS region were compared between the ROM1 predictions and the observations at surface monitoring sites, to the extent that these sites could define such plumes.

The daily maximum O_3 concentration, c(max,ob), at a measuring site can be compared with the corresponding model prediction in two different ways. First, the predicted maximum at the site, c(max,p0) for ROM1 layer 0 or c(max,p1) for layer 1, can be compared to c(max,ob) (paired in space). Second, a more restrictive measure matches the prediction that occurs at the same hour as the

observed maximum with the observed concentration [c(p0,h(ob)) vs. c(max,ob) and c(p1,h(ob)) vs. c(max,ob); paired in space and time].

A summary of average concentration data from the daily maximum values analysis for the model simulation is presented in Table 1. Results from the full data set, as well as the data subset where all O_3 concentrations are greater than 50 ppb, are given. The number of receptor stations dropped from 156 in the full data set to 47 in the data subset. Interestingly, the average observed maximum value increased by only 2 to 4 ppb from the data set to the subset because there were very few observed <50-ppb maxima at the monitoring site locations. Conversely, the average model predictions increased by 20 to 30 ppb from the data set to the subset because of the large number of values near the background O_3 level. This is the reason for the large drop in the number of stations in the data subset. For the comparison of observed and predicted maximum values paired in space, the average bias at all receptor sites was 24.8 ppb on 3 August, representing a 34% underprediction and 25.3 ppb on 4 August, representing a 33% underprediction for model layer 0. For layer 1, the corresponding values were 23.2 ppb (32% underprediction) on 3 August, and 23.3 ppb (30% underprediction) on 4 August. In the data subset where the lower O_3 values are excluded, the results show a marked improvement. On 3 August, the average bias for layer 0 was 11.3 ppb (15% underprediction) and on 4 August, it was 5.6 ppb (7% underprediction). For layer 1 the corresponding values were 9.2 ppb (12% underprediction) on 3 August, and 2.7 ppb (3% underprediction) on 4 August.

Table 1. Summary of ROM1 results for daily O_3 maximum values analysis.*

	Full Data Set		Data Subset (all concentrations > 50 ppb)	
	79215	79216	79215	79216
Number of stations	156	154	47	48
Average c(max,ob)	73.2	77.8	75.5	81.8
Average c(max,p0)	48.4	52.5	64.2	76.2
Average c(p0,h(ob))	40.0	43.5	60.0	68.9
Average c(max,p1)	50.0	54.5	66.3	79.1
Average c(p1,h(ob))	41.6	45.1	62.0	71.4

*All concentrations are in ppb.

The plume maximum values analysis is performed to isolate for comparison individual areas or plumes of high O_3 concentrations from the model predictions and the ambient observations. The perspective of this analysis is broader than that of the daily maximum values analysis in that model predictions at the same location as the observation are not necessarily required. Instead, the eligible area from which the model prediction is chosen is defined to be the coherent region of concentrations, or plume, from which the observation comes. This less restrictive pairing permits us to match observations and predictions based on supposedly similar phenomenological events in the physical processes producing the maximum O_3 values. It also allows for possible transport errors in plume definition. This perspective also permits us to include a larger area than the single site location where the maximum value occurred.

In estimating model performance in terms of the plume maximum perspective, three different comparisons of model-predicted concentration with the maximum observed concentration, c(max,ob), in the O_3 plume are made. First, the maximum observed concentration was compared with the predicted maximum at the same location as the monitoring site of the observed maximum (paired in space). Second, the observed maximum was compared with the predicted concentration at any of the monitoring site locations in or near the projected plume (unpaired in space; site to site), and finally it was compared with the maximum concentration found in the grid cell at the center of the projected O_3 plume (unpaired in space; site to grid cell). These three values are designated (for ROM1 layer 1) as c(max,p1-A), c(max,p1-B), and c(max,p1-C), respectively, and proceed from the most to the least strict pairing of concentrations in the plume maxima analysis.

The bias expected from the A comparison (paired in space) is the greatest among the three types of pairings. This is the most severe test for an air quality model and usually model performance for O_3 indicates an underprediction in this case. The B comparison (unpaired in space; site to site) constitutes the most neutral test of the three. It is possibly the best estimate of the actual bias of a model. All other factors being equal, the chances of an under- or overprediction here are about even. The C comparison (unpaired in space; site to grid cell) has the greatest potential for overprediction because the density of stations in a measurement network is rarely sufficient to capture the true O_3 peak value.

Table 2 presents a summary of statistics from the analysis of O_3 plume maximum values. Seven individual plumes were considered. The average value of c(max,ob) recorded at surface monitoring sites in these plumes was 114.9 ppb. Three methods of pairing this observed value with ROM1 predictions were made. From the most restrictive to the least restrictive pairing the corresponding layer 1 model predictions averaged over the 7 cases were c(max,p1-A) = 87.3 ppb, c(max,p1-B) = 106.9 ppb, and c(max,p1-C) = 151.0 ppb. The last predicted value is not restricted to measurement site locations, but can be at any grid cell within the predicted plume area. The average bias for this pairing was -36.1 ppb, implying an average overprediction of about 31%.

The average bias in the most restrictive pairing for which the model prediction is interpolated to the same location as the monitoring station was 27.6 ppb, and the corresponding degree of underprediction was 21.6%. For the second comparison, whereby the maximum model prediction was restricted to monitoring site locations in or near the O_3 plume, but not necessarily at the site of the observed maximum, the average bias was 8.0 ppb with a corresponding degree of underprediction of 4.4%. This may be the best estimate of the model bias for the plume analysis.

Table 2. Summary of ROM1 results for plume O_3 maximum values analysis.*

Urban Plume	Date	C(max,obs)	C(max,p1-A)	C(max,p1-B)	C(max,p4-A)
Detroit	3 Aug.	120	90	122	158
Toronto	3 Aug.	98	110	110	144
New York	3 Aug.	130	97	97	117
Detroit	4 Aug.	99	98	94	162
Toronto	4 Aug.	101	66	107	227
New York	4 Aug.	144	59	88	114
Philadelphia	4 Aug.	132	101	130	135
Average		115	87	107	151
S.D.		20	18	15	38

*All concentrations are in ppb.

4. CONCLUSIONS

The first generation U.S. EPA ROM1 has been evaluated for O_3 concentrations using the 2-day test period, 3-4 August 1979, from the NEROS data base. In the stage of the evaluation where all data were involved, results showed that, on the average the ROM1 underpredicted O_3 levels by 6% in comparison with measurements at monitoring sites. In a second part to the analysis, the bias was examined for a subset of the data where only simultaneous O_3 values above 50 ppb were included for observed and predicted concentrations at monitoring sites. In this case, the average ROM1 performance for the data subset showed a 4.6% underprediction for layer 0 and a 1.4% underprediction for layer 1.

The second aspect of model evaluation, using daily O_3 maxima, also proceeded in 2 steps. In the first step, the daily maximum value at each receptor location was compared to the predicted maximum at that location as well as the prediction made for the same time as the observed maximum, the more stringent comparison. For layer 1, the ROM1 performance showed an average 31% underprediction for the first comparison and a 43% underprediction for the second comparison. Results for layer 0 were similar. When data were restricted to those observed and predicted O_3 pairs above 50 ppb, the model performance for the daily maximum analysis improved by showing average underpredictions of 8% and 15%, respectively, for the above layer 1 comparisons. The improvement in model predictions in this case was primarily due to restricting the analysis to comparisons at monitoring station locations that were most affected by source emissions.

The second step of evaluating the ROM1's performance for O_3 maxima predictions involved an analysis of individual plumes of O_3 from major source areas within the NEROS region. Seven cases of such plumes were identified and analyzed for the 3-4 August 1979 episode. The evaluation used three types of comparisons of O_3 maxima ranging from a strict spatial pairing between observed and predicted values to a fairly loose spatial pairing. Results averaged over the 7 plumes in the test case showed a 22% underprediction for the strictest paired comparison, a 4% underprediction for the intermediate comparison, and a 38% overprediction for the loosely paired comparison. We may judge the model performance to be quite good for maximum O_3 levels in the vicinity of O_3 plumes (4-22% underprediction). The 38% overprediction for the loosest spatial pairing is an exaggeration of model performance; overprediction is expected in this unpaired type of comparison. Applications with the second generation regional model, ROM2, should be able to quantify the model performance to a greater degree than was done here with the first generation model.

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